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Work involved theoretical interpretation of measured absorption spectra of atoms in electric and magnetic fields. Fourier-transformation of the absorption spectrum produces what we call the "Recurrence Spectrum." It consists of a series of sharp peaks, and each peak is correlated with a "recurrence": an electron orbit that goes away from the atom and later returns. We derived general formulas that relate measured recurrences to properties of classical electron orbits and quantum wave-functions. Good agreement was found between this theory and experiments. More refined experiments showed bifurcation and proliferation of recurrences correlated with the transition from orderly to chaotic motion of the electron. Classical bifurcation theory was extended and adapted to describe these phenomena.

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II. FINAL TECHNICAL REPORT
RESULTS OF PRIOR ONR SUPPORT

A. Scaled Variables Experiments and Bifurcations of Closed Orbits

Central to our recent work has been the interpretation of scaled-variables experiments carried out by the Bielefeld group.[10a] It was known that the classical Hamiltonian for a Hydrogen atom in a magnetic field obeys a scaling law. This scaling law asserts that the shapes of trajectories do not depend upon the energy and magnetic field separately, but only upon the scaled energy $\epsilon = EB^{-2/3}$. Furthermore, at each fixed ϵ, the size of any orbit changes with B such that the classical action is proportional to $B^{-1/3}$. With this in mind, the Bielefeld group measured absorption vs. $B^{-1/3}$, varying the photon energy and magnetic field simultaneously to keep $EB^{-2/3}$ fixed. One result is shown in Fig. 2, and is compared to the results of closed orbit theory. As expected, theory accurately accounts for

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the observations. Each observed peak in the Fourier transform of the absorption spectrum is correlated with a closed orbit, or with a cluster of closed orbits having similar classical actions. We call a plot like that in Fig. 2 a "Recurrence Spectrum."

In Fig. 3, recurrence spectra at many different scaled energies are drawn in a single picture. At low scaled energies, only a few recurrences are present. As the scaled energy increases, recurrences proliferate, and individual peaks split into mountain ranges. The observed proliferation of recurrences reminds us of the work of Feigenbaum and others,[12,13] who showed that the logistic map has a sequence of period-doubling bifurcations with "universal" properties. We found that this "universal" sequence is not visible in the experimental data, but it is evident that some other patterns are present.

In the present context, a "bifurcation" is the creation of a new periodic orbit or the splitting of one periodic orbit into several. After much study of bifurcation theory, we came across a little-known paper by K. Meyer, a mathematician now at the University of Cincinnati.[14] This paper showed that there are precisely five "generic" forms of bifurcation in Hamiltonian systems. We call them saddle-center bifurcations, period-doublings, 3-touch-and-go bifurcations, 4-touch-and-go or 4-island-chain bifurcations, and 5-and-higher-island chain bifurcations (Fig. 4). "Generic" means that other types can exist, but they would be atypical--they would happen only "accidentally," or in the presence of some special symmetry. In fact, our system has a number of symmetries: time reversal invariance, and reflection symmetries about the ρ- and z-axes. We examined the consequences of these symmetries, and we showed that in certain cases the structure of bifurcations is modified by the presence of these symmetries.

This general framework provides a logical structure for interpretation of the observations. We have shown that: (1) the "exotic" orbits discovered in ref. 10 are produced by saddle-center bifurcations; (2) a sequence of pitchfork and period-doubling bifurcations produces the "main sequence"; (3) both generic (touch-and-go) and special (island chain) period-triplings produce some of the peaks that are visible in the experiment; (4) a focusing effect associated with a 4-island-chain bifurcation is also visible. One paper on the general theory of bifurcations and on the specific bifurcations that occur in this system was published in 1992,[15a], and a second, giving a detailed comparison between theory and experiment,[15b] was published early in this grant cycle.

This analysis and comparison with experiment constitutes a significant advance for bifurcation theory in Hamiltonian mechanics: I know of no other observations on conservative systems in which whole families and sequences of bifurcations appear so naturally in experimental measurements. This theory also advances our knowledge of quantum chaology: we are seeing the transition from order to chaos in a new way. It helps to emphasize the central role of periodic-orbits in the study of chaotic systems. Finally, it provides a new but natural framework for interpretation of atomic and molecular absorption spectra.

B. An Advance in Bifurcation Theory

As we explained earlier, Meyer's theorem lists five "generic" bifurcations. These are the types that occur "typically" in systems with two degrees of freedom under variation of a single parameter. (Again, "typical" or "generic" means that other things can happen, but only "accidentally" or in the presence of a symmetry.) Here is an area where atomic spectroscopy simulates advances in classical mechanics. Atoms in electric and magnetic fields can have two or three degrees of freedom, there are two continuously variable parameters (F and B), and there are symmetries that can be broken (for example cylindrical symmetry in parallel fields can be broken by varying the angle between F and B).

(a) What bifurcations are generic under the symmetries that commonly occur in an atomic system? We analyzed what we saw, but a more systematic development is needed that will cover all the cases that commonly occur.

(b) What bifurcations are generic in two degrees of freedom if two parameters are available? This is the mathematicians' way of formulating an interesting question about classical mechanics. Physicists think in terms of specific examples. For an atomic electron in a magnetic field pointing in the z direction there is an orbit that lies in the xy plane (the "quasi Landau" orbit producing the oscillations first seen by Garton and Tomkins). This orbit undergoes (among other things) pitchfork bifurcations. However this bifurcation is non-generic because of reflection symmetry between $\pm$ z. Applying an electric field breaks the $\pm$ z symmetry, and we would expect it to convert the bifurcation into one of the generic types. The focusing properties and the observed effects in the recurrence spectrum must then be changed. The list of bifurcations that are generic under variation of two parameters must include this kind of reflection-symmetry-breaking phenomenon.

(c) What bifurcations are generic in three degrees of freedom if two parameters are available? Is it the same list? Again atomic spectroscopy forces us to address this question. The orbit parallel to the magnetic field has non-generic bifurcations that would be modified if a perpendicular electric field were added. At the same time the number of important degrees of freedom changes from two to three.

I had the good fortune to meet Ken Meyer at a conference recently. After explaining to him our work, the application of his theorems to atomic spectroscopy, and the questions in our minds, he went home and dug out some old notes on generic two-parameter bifurcations. (He had looked at the mathematical problem years ago, but had thought no one would be interested.) He suggested we write a joint paper[15i] on this subject, combining the general theory with calculations on atoms. In this paper he evaluated two generic cases of two-parameter bifurcations, and showed the patterns that occur. In particular he showed how a pitchfork bifurcation, which occurs in the presence of a symmetry, splits into a saddle-node bifurcation if the symmetry is broken.

With this analysis available, we re-examined the pitchfork bifurcation of the "quasi-Landau orbit." The results surprised us. Application of a symmetry-breaking electric field parallel to the magnetic field did not destroy the pitchfork structure of the bifurcation. This non-generic bifurcation is present because of "hidden symmetries" associated with Coulomb problems. Clearly we have a lot more to learn. We will return to this topic in section III.A.1.

These theoretical developments in classical mechanics will guide future experiments on atoms in parallel or in crossed fields. Presently there are at least four experimental groups having the interest and capacity to carry out the relevant scaled-variables experiments, in Bielefeld, Amsterdam, Munich and Cambridge. We are in close contact with all of them, and we discuss with them prospects for appropriate measurements.

C. Normal Forms and the Organization of Sequences of Bifurcations

In studying the bifurcations of orbits in the diamagnetic Kepler problems we found that there was a commonly-occurring pattern. Certain of the generic bifurcations classified by Meyer were occurring in a regular, organized sequence. In particular, we examined the bifurcations that produce an orbit that we like to call "pac-man." This is a period-4 bifurcation, and one of the expected forms of such bifurcations is what we call an "island-chain": Four stable PO's (O points) and four unstable PO's (X points) move toward the central stable PO, collide with it simultaneously, and disappear, leaving the central PO stable.

We saw this phenomenon in our calculations, but we saw that it was part of a more complicated sequence of events (Fig. 5): (a) A stable-unstable pair of period-4 orbits was created nearby in a "saddle-node" bifurcation. (b) A second such pair was created in a similar fashion. (c) The separatrices rearranged into two concentric four-island chains. (d) The actual period-4 bifurcation of Meyer's theorem occurred: the inner chain shrank and collapsed onto the perpendicular orbit, leaving only the outer chain. All these observations came out of careful examination of many numerical calculations; at the time, we could neither anticipate nor explain such sequences of events. We observed, however, that most of the bifurcations of the perpendicular orbit occur through such ordered sequences. We have reasons to believe that these ordered sequences occur in many systems.

Normal-form theory is a systematic procedure for locally converting the original Hamiltonian having two degrees of freedom into an effective Hamiltonian having only one degree of freedom. The effective Hamiltonian is a power series in (p,q); we find that it describes bifurcations in the greater neighborhood of the original PO, and it describes the sequential organization of these bifurcations.

Normal-form theory is an old subject in mathematics. It has its origins in the work of Birkhoff in 1926, and the theory provides the proof of Meyer's theorem about generic bifurcations of periodic orbits. It has usually been used as a tool for qualitative analysis,

describing what can happen in dynamical systems. Mathematicians have long known that normal-form theory could also be a tool for quantitative analysis--what does happen in a particular system, at what values of parameters. We first introduced normal-form theory as a tool for semiclassical mechanics in 1979.[15q] We were studying energy eigenvalues of the Henon-Heiles system, and we showed that the normal-form expansion about an equilibrium point provides a reasonable approximation to and a semiclassical interpretation of all the eigenvalues (despite the presence of chaos).

Normal-form theory for displacements from a periodic orbit is similar to the theory for displacements from equilibrium, but normalization about a periodic orbit is a far more complicated process; Arnold calls it one of the "most complex problems of bifurcation theory." Even after the theory is worked out in principle, a lot of creativity is required to implement the theory computationally.

Happily I got a postdoc who was well-trained in the Russian school of mathematics, and he was not only able to master all the required theory, but he invented a means for implementing it. We believe our calculation is the first full development and implementation of normal-form theory as a quantitative tool for analyzing bifurcations of periodic orbits.

The final result of the theory is a smooth function of two variables and one parameter; external-points and saddle-points of this function correspond to the stable and unstable periodic orbitsof the system. As the parameter is varied, it is easy to understand the sequence of creation and destruction of extrema and saddles. With this understanding, we obtain an interpretation of the sequence of creation and destruction of periodic orbits. A brief description was published in Phys. Rev. Letters,[15n] and an extensive description of the theory is now accepted in Phys. Rev. E.

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D. Electron Detachment in Parallel Electric and Magnetic Fields

Electron detachment from a negative ion $h\nu + H^- \rightarrow H + e^-$ is in some ways simpler than excitation or ionization of a neutral atom because there is no long-range Coulomb force affecting the active electron. If detachment takes place in parallel electric and magnetic fields, then the Hamiltonian governing the motion of the detached electron is

$$H = \frac{p^2}{2m} + eFz + \frac{e^2B^2}{8mc^2}\rho^2$$

We have uniform acceleration down the z-axis and circular cyclotron motion in (xy), which is equivalent to harmonic oscillation in ρ. This is, therefore, a very simple system, but it has keys that unlock solutions to a number of problems. (1) The relevant parts of the model are exactly solvable. Whereas the mathematical theory of bifurcations is very abstract, everything in the present system can be understood by elementary methods. (2) It admits a simple structure of closed orbits and their associated recurrences, and it possesses an orderly sequence of bifurcations. (3) At each bifurcation a certain geometrical structure--a cylindrically focused cusp--passes through the origin. This causes the semiclassical approximation to fail. (4) The failure is repaired by a simple diffraction function, a Fresnel integral. The integral provides a uniform approximation which is always finite and which behaves correctly in all limiting cases. (5) The focused cusp is sufficiently similar to the structures found in excitation of neutral atoms that the present model has helped us to derive appropriate formulas for those more difficult cases. (6) Finally, the model accurately represents a system on which experimental measurements can test the predictions.

We calculated closed orbits for this system, and their associated recurrence-strengths, we found the energies at which the semiclassical formulas diverge because of bifurcations, and we derived and used Fresnel-integral formulas to correct these divergences (Fig. 6). A preliminary report was published in Phys. Rev. Letters,[15f] and two papers presenting the full details are submitted to Phys. Rev. A.

E. Ionization of Alkali Atoms in Electric Fields

Stimulated by experiments of groups led by Gallagher, by Metcalf, and by Welge[16,17], graduate student J. Gao used closed orbit theory to describe ionization and excitation of sodium in electric fields[15e]. Electric fields are easy because (excluding core effects) the Schröedinger equation is separable in parabolic coordinates. Furthermore, above the zero-field ionization threshold, there is only one closed orbit of the electron; it goes straight up against the electric field and then returns to the atom. The more challenging aspect involved incorporation of spin-orbit coupling and core effects. The quantum defect produces a small phase-shift to the outgoing and returning waves, and spin-orbit coupling in the initial state ($3p\ ^2P_{j=3/2}$) modifies the angular distribution of the outgoing waves. Two papers were published on this subject during the previous grant cycle.

More interesting phenomena occur below the ionization threshold. The parallel orbit undergoes a sequence of bifurcations, sending out additional closed orbits. We predicted exactly where these bifurcations should occur, and what their effects should be.[15f] The recurrence-strength of the nth-repetition of the parallel orbit should get very large near a bifurcation. Indeed, semiclassical formulas for the recurrence-strength again diverge at a bifurcation, and have to be repaired. The divergence again results from the passage of a focused-cusp through the origin, and the repair of the divergence is similar to the theory developed for detachment (section D above).

After we had predicted the energies at which bifurcations occur, and while we were developing our formulas to correct the divergences, experimental measurements in Dan Kleppner's group came online. We were able, therefore, to test our formulas directly against their measurements. We got good agreement between theory and experiment. This was published in Phys. Rev. Letters,[15m] and a detailed paper is submitted to Phys. Rev. A.

F. Scattering of Electrons by the Ion Core

When the active electron travels around a closed orbit and returns to an alkali ion, it feels both the Coulomb field and a short range field within the core of the residual ion. This short-range field produces and phase-shifts in the lower partial-waves (related to quantum defects in the energy levels). The result is that the electron wavefunction splits into a superposition of a Coulomb-scattered part (which scatters backwards to retrace the original orbit) and a core-scattered part, which is approximately spherical, and which produces outgoing waves on every other orbit.

In our 1992 paper, Gao described core-scattering and its effects,[15e] and in her calculations, showed that these effects were too small to be visible in the experiments we were then analyzing. Later, experimental measurements and quantum calculations of recurrence spectra at MIT and in Paris found visible effects of core-scattering. Recently, Dando et al.[19b] put Gao's formulas into more explicit form, and showed that these semiclassical formulas give an accurate description of core-scattering. The core produces "shadows" on the original orbit, reducing the recurrence-strength associated with subsequent repetitions of the orbit, and it produces combination-recurrences, in which the electron is scattered from one closed orbit to another (Fig. 7).

G. Action of a Half-Cycle Pulse on an Atomic Electron in a High Rydberg State

In 1993 Bucksbaum's group at Michigan found a way to apply a very short approximately-DC electric pulse to an electron in an atom in a Rydberg state. They called it a half-cycle pulse (HCP). We have proposed and studied theoretically a modification of their experiment, in which both a static electric field and the HCP act on the electron.[15o] We used a one-dimensional model to calculate the transition probability from one "red" Stark state to another, and from one "blue" Stark state to another. It is easy to show that in general an even number of trajectories connect the initial state to the final state. Therefore

an interference pattern should be visible in the transition probability as a function of n or as a function of the strength of the applied field. We also showed the existence of a threshold-field at which the number of trajectories from initial state to certain final states changes from two to four (yet another bifurcation). Such measurements are now going on at University of Virginia.